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14. ABSTRACT
The objeetive of this proposal is to support a symposium on using modern theoretical mechanics theories to discover new materials. Examples inelude low-hysteretie media whieh would revolutionize aetuators and ferromagnetie shape-memory alloys whieh would provide interesting, reeonfigurable antennas. The organizers will sehedule both individual speakers from among the world's leading experts and foeused multi-speaker sessions. The AF antieipates using designed materials to aehieve greater funetionality of its inventory.

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Final Report on Grant AFOSR FA9550-08-1-0371 used to organize:

Symposium on Using Mechanics to Discover New Materials
45th Annual Technical Meeting of the Society of Engineering Science
October 12-15, Urbana-Champaign

Principal Investigator:
Kaushik Dayal, Carnegie Mellon University

Program Manager:
Arje Nachman, Air Force Office of Scientific Research

Symposium Organizers:
Kaushik Bhattacharya, California Institute of Technology
Kaushik Dayal, Carnegie Mellon University
Antonio DeSimone, SISSA, Italy

Background

The recent years have seen numerous examples where mechanics, in conjunction with systematic mathematical analysis and large-scale computation, has played a critical role in the discovery, development and improvement of new materials. The discovery of extra-ordinarily large strain in ferromagnetic shape-memory alloys, the discovery of new shape-memory alloys with ultra-low hysteresis, morphological instabilities in thin films and development of new quantum dot structures are but a few examples. However, each problem has created its own small community and the endeavors have been largely disconnected from each other. With the growing list of successes and the growing communities, the time is ripe to have a systematic discussion about creating a broader approach wherein the diverse groups can learn from each other and new problems can be tackled. This symposium successfully created a forum for this discussion.

Symposium

This symposium highlighted how mechanics across scales ranging from angstroms to meters has enabled the improvement of existing materials and the discovery of new materials. It brought together speakers from diverse disciplines including mechanics, mathematics and materials science and backgrounds ranging from academics to industry and working on diverse problems. The breadth of this symposium can be gauged by the range of exciting topics, including:

- Texture and grain growth
- Thin film mechanics
- Fundamental issues in elasticity, including symmetry, the Eshelby problem, and minimum principles for rate problems
- Control devices using shape-memory alloys
- Covalent bonding in biological systems, the mechanics of viruses and human organs, and the use of mechanics in vascular NiTi stent design
- Homogenization theory for dynamic linear continuum systems and shape-memory honeycomb structures

- Experiments, modeling and simulation on the mechanics of advanced materials, including carbon nanotubes, shape-memory alloys, thermoplastic elastomers, ferromagnetic shape-memory alloys, and piezoelectrics
- Analysis and application of quasicontinuum methods

The talks described various examples and contemporary methods of analysis, computation and experiments that have been brought to bear on this subject, and set the stage for broad-ranging discussions.

This symposium was organized as a part of the 45th Annual Technical Meeting of the Society of Engineering Science and was held in honor of Richard D. James, winner of the 2008 Prager Medal.

The list of speakers is in Appendix A, and the abstracts that have been extracted from Conference Materials in Appendix B.

Disbursement of Funds

The speakers are active and recognized researchers in the field, and therefore the organizers anticipated that a majority of them will be able to obtain other sources of funds to attend this symposium. At the same time, organizers of the symposium sought to bring together researchers at various stages of their careers, in particular to draw from the experience of very senior researchers and to inspire a selected group of early-career researchers. The AFOSR funds were used to support the hotel and registration expenses of 5 early-career researchers, and to support the registration expenses of 1 senior researcher.

Appendix A: List of Speakers
Symposium on Using Mechanics to Discover New Materials
45th Annual Technical Meeting of the Society of Engineering Science
October 12-15, Urbana-Champaign

In order of presentation:

1. David Kinderlehrer, Carnegie Mellon University
2. Irene Fonseca, Carnegie Mellon University
3. Scott J. Spector, Southern Illinois University
4. Raffaella Rizzoni, University of Ferrara
5. Liping Liu, University of Houston
6. L. Ben Freund, Brown University
7. William S. Klug, University of California Los Angeles
8. Isaac Chenchiah, University of Bristol
9. Rodney Clifton, Brown University
10. John Willis, University of Cambridge
11. Graeme Milton, Utah University
12. Michael Ortiz, California Institute of Technology
13. Traian Dumitrica, University of Minnesota
14. Kaushik Dayal, Carnegie Mellon University
15. Mitchell Luskin, University of Minnesota
16. Pedro Ponte-Castaneda, University of Pennsylvania
17. Valery Levitas, Iowa State University
18. Ellad Tadmor, University of Minnesota
19. Anja Schlomerkemper, Max-Planck Institute
20. Ichiro Takeuchi, University of Maryland
21. Doron Shilo, Technion
22. Ryan Elliott, University of Minnesota
23. Pradeep Sharma, University of Houston
24. Nicolas Triantafyllidis, University of Michigan
25. Timothy Healey, Cornell University
26. Dominique Schryvers, Antwerp University
27. Brian Berg, Boston Scientific Inc.

Appendix B: Presentation Abstracts (extracted from Conference Materials)
Symposium on Using Mechanics to Discover New Materials
45th Annual Technical Meeting of the Society of Engineering Science
October 12-15, Urbana-Champaign

Prager Medal Symposium in Honor of Richard James: Using Mechanics to Discover New Materials

SYMPOSIUM D

ORGANIZERS:

Kaushik Bhattacharya, *Division of Engineering and Applied Science, California Institute of Technology*

Kaushik Dayal, *Carnegie Mellon University*

Antonio DeSimone, *SISSA*

New Perspectives on Texture Evolution

David Kinderlehrer
Professor
Mathematical Sciences, Carnegie Mellon University

Shlomo Taasan
Professor
Mathematical Sciences, Carnegie Mellon University

Nearly all technologically useful materials are polycrystalline, consisting of small crystallites, called grains, separated by interfaces, the grain boundaries. The energetics and arrangement of this network, its texture, are important factors in material behavior, and constitute the basic problem of microstructure. Experimentally, the inverse relationships between grain boundary populations and energy have been observed for many years. We introduce the grain boundary character distribution (GBCD), a new statistic, and offer compelling evidence for its strong dependence on grain boundary energy. In addition we demonstrate that there are natural laws for texture and the GBCD using large network simulations. This is joint work with the MIMP group at Carnegie Mellon University.

Equilibrium Configurations of Epitaxially Strained Crystalline Films: Existence and Regularity Results

Irene Fonseca
Department of Mathematical Sciences, Carnegie Mellon University

Strained epitaxial films grown on a relatively thick substrate are considered in the context of plane linear elasticity. The total free energy of the system is assumed to be the sum of the energy of the free surface of the film and the strain energy. Due to the lattice mismatch between film and substrate, flat configurations are in general energetically unfavorable and a corrugated or islanded morphology is the preferred growth mode of the strained film. New regularity results for volume constrained local minimizers of the total free energy are established, leading to a rigorous proof of the zero contact-angle condition between islands and wetting layers.

On the Symmetry of Energy Minimizing Deformations in Nonlinear Elasticity: Compressible Materials

Scott J. Spector
Professor of Mathematics
Department of Mathematics, Southern Illinois University

Jeyabal Sivaloganathan
Reader in Mathematics
Department of Mathematical Sciences, University of Bath

Consider a homogeneous, isotropic, hyperelastic body that occupies a three-dimensional, thick spherical shell, S, in its reference state and is subject to radially symmetric displacement boundary conditions on its inner and outer boundaries. It is shown [1,2] that, to each deformation of the shell, there corresponds a radial deformation that has less elastic energy than the given deformation, whenever the stored-energy function is polyconvex and grows sufficiently rapidly at infinity.

The key ingredient is a new radial-symmetrization procedure that is appropriate for problems where the symmetrized mapping must be one-to-one in order to prevent interpenetration of matter. The radial symmetrization of an orientation preserving diffeomorphism, u:S—>S*, between shells S and S* is the radial deformation

$v(x)=(R(r)/r)x$, where $r=|x|$,

that maps each sphere Sr of radius r>0, centered at the origin into another such sphere that encloses the same volume as u(Sr). Since the volumes enclosed by the surfaces u(Sr) and v(Sr) are equal, the classical isoperimetric inequality then implies that the surface area of u(Sr) is bigger than the surface area of v(Sr). The equality of the enclosed volumes together with this reduction in surface area is then shown to give rise to a reduction in total energy for many of the constitutive relations used in nonlinear elasticity.

These results are also extended to classes of Sobolev deformations and applied to prove that the radially symmetric solutions to these boundary-value problems are global energy minimizers in the class of (possibly non-symmetric) deformations of a three-dimensional thick spherical shell.

References

[1] J. Sivaloganathan, S.J. Spector, Http://www.math.siu.edu/spector/incompressible.pdf

[2] J. Sivaloganathan, S.J. Spector, Http://www.math.siu.edu/spector/compressible.pdf

Shape Control of Polymeric Sheets Using SMA Wires

Dr. Raffaella Rizzoni
Department of Engineering, University of Ferrara

Mattia Merlin
Department of Engineering, University of Ferrara

We investigate, both from an experimental and a theoretical point of view, the behavior of SMA composites fabricated by bonding thin pre-deformed SMA wires to a polymeric matrix. The motivation of this study is primarily the design of a structure changing shape to change operating characteristics. Some relevant material properties are experimentally determined. A large number of tests are carried out on Ti-50.5at.%Ni wires, in order to describe the stress-temperature and the strain-temperature relations. In particular, the transformation temperature ranges of the wires are obtained via differential scanning calorimetry (DSC) tests and the latent heats on heating and cooling are calculated. The elastic moduli of the martensite and austenite phases are

determined by tensile tests at low and high temperatures. Constant stress tests and constrained recovery tests are also performed, in order to determine the relation between stress and the transformation temperatures, and the maximum recovery stress, respectively. The mechanical properties of the polymeric matrix are also studied. To simulate the behavior of the composite, a simple model is presented, which assumes classical plate theory for the composite. The behavior of the SMA wires is described by the theory for heterogeneous thin wires developed in [2], which, using ideas of the constrained theory of martensite [1], is specialized to phase transforming materials with high elastic moduli [3]. Simulations of the composite change of shape for different arrangements of the SMA wires are given. Experimental results on an epoxy resin composite plate with SMA embedded wires are also presented, showing that an appreciable bending can be obtained during wires activation.

References

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[2] H. Le Dret and N. Meunier, (2005), Modeling heterogeneous martensitic wires, Math. Models and Meth. Appl. Sci., 15, 3, 375—406.

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Solutions to the Periodic Eshelby Inclusion Problem in Two Dimensions

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Postdoc
California Institute of Technology

We consider the classic Eshelby inclusion problem on a finite unit cell with periodic boundary conditions. We give solutions in terms of Cauchy-type integrals to this problem in two dimensions for general shapes of inclusion and nonuniform but divergence-free eigenstress. This representation formula is reminiscent of the familiar Greens representation formula. More, it is shown that a Vigdergauz structure does not have the Eshelby uniformity property for non-dilatational uniform eigenstress unless it degenerates to a simple laminate.

Modeling the Forced Separation of a Molecular Bond

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Interest in this topic derives from the observed behavior of the non-covalent molecular bonds that account for adhesion of eukaryotic animal cells to extracellular matrix [1]. For purposes of modeling, bonding is understood to be the confinement of the configuration of the the system within an energy well, which arises as a principal feature of an overall energy landscape [2]. One consequence of application of a force on the bond is to distort this landscape over time. The system functions in a thermal environment, and the depth of the bond well is assumed throughout to be significantly greater than the thermal energy unit kT. The bond state is characterized by a probability distribution over the energy landscape and, as the landscape distorts, its evolution is governed by a partial differential equation. The system is analyzed in order to extract information on the most probable time for bond separation, the maximum force that can be sustained by the bond, and the sensitivity of bond separation behavior to loading rate, for example. The goal of experiments in which molecular bonds are separated under force is to infer magnitudes bond characteristics. The purpose of this discussion is to consider the relationships between measured quantities and properties of the bond itself, as modulated by an intervening loading apparatus [3].

References

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[2] P. Hanngi, P. Talkner and M. Morkovec, Reaction-rate theory: Fifty years after Kramers, Reviews of Modern Physics 62, 251-342, 1990.

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Modeling the Mechanics of Viral Capsids

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Melissa M. Gibbons
Graduate Student
Department of Mechanical and Aerospace Engineering, University of California, Los Angeles

Lin Ma
Graduate Student
Department of Mechanical and Aerospace Engineering, University of California, Los Angeles

As revealed by techniques of structural biology, the protein shells of viruses (capsids) are some of natures most beautiful and robust examples of highly symmetric multiscale self-assembled structures. The ability of viral capsids to respond structurally and mechanically to physical and chemical stimuli also gives them tremendous potential as components for the design of synthetic materials with adaptive properties, as has been demonstrated recently by the creation of virus-based nanowires. A series of recent indentation experiments using atomic force microscopy (AFM) has shown that capsids also possess impressive mechanical properties of strength and elasticity. In this talk I will present some theory and numerical modeling of viral capsids based on continuum mechanics and Ginzburg-Landau theory of phase transitions, and I will discuss what weve learned about the elastic response and mechanical failure of viral capsids, and coupling of global capsid mechanical response to local protein conformational change. Overall the talk will highlight our ongoing efforts to push the limits of usefulness of continuum theory via coupled continuum-atomistic multiscale modeling of capsids and other large protein assemblies.

A Model for T4 Tail Sheaths

Isaac Chenchiah
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Department of Mathematics, University of Bristol

Valeriy Slastikov
Lecturer
Department of Mathematics, University of Bristol

Building on the insights of Falk and James [1] we present a model for bacteriophage T4 tail sheaths. The model predicts helical configurations, phase transitions and non-uniform states—these are analysed and compared with experiments.

Reference

[1] Falk, W and James, R. D., Elasticity theory for self-assembled protein lattices with application to the martensitic phase transition in bacteriophage T4 tail sheath, Physical Review E 73(1), 011917 (2006)

Effective Relations for Inhomogeneous Elastodynamics and Electrodynamics

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The theory underlying effective constitutive relations for inhomogeneous elastodynamics is largely complete, even though there may remain practical difficulties in implementation. In contrast, there appears still to be some resort to ad hoc prescription in the case of inhomogeneous electrodynamics, even in the "homogenization limit". The purpose of this talk will be to follow, as faithfully as possible, a route recently developed and explored for elastodynamics [1,2], in the context of electrodynamics, to establish correspondences and differences and perhaps improve thereby appreciation of the structure of electrodynamic effective relations.

References

[1] G.W. Milton, M. Briane and J.R. Willis, "On cloaking for elasticity and physical equations with a transformation invariant form". New J. Physics 8 (2006), 248.

[2] G.W. Milton and J.R. Willis, "On modifications of Newton's second law and linear continuum elastodynamics". Proc. R Soc. A 463, (2007), 855-880.

Minimization Variational Principles for Acoustics, Elastodynamics, and Electromagnetism in Lossy Inhomogeneous Bodies at Fixed Frequency

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The classical energy minimization principles of Dirichlet and Thompson are extended as minimization principles to acoustics, elastodynamics and electromagnetism in lossy inhomogeneous bodies at fixed frequency. This is done by building upon ideas of Cherkaev and Gibiansky, who derived minimization variational principles for quasistatics. In the absence of body forces the primary elastodynamic minimization variational principles have a minimum which is the time-averaged elastic energy dissipated to heat in the body. The variational principles provide constraints on the boundary values of the fields when the moduli are known. Conversely, when the boundary values of the fields have been measured, then they provide information about the values of the moduli within the body. This should have application to tomography. We also derive saddle point variational principles which correspond to variational principles of Gurtin, Willis, and Borcea.

Minimum Principles for the Trajectories of Systems Governed by Rate Problems

Michael Ortiz
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The evolution of many physical systems is the result of a balance between dissipative and energetic forces. This balance results in evolutionary equations that govern the time-dependence of the state of the system. The classical treatment of these equations tends to break down when applied to strongly nonlinear systems that develop evolving microstructures. In these cases, the energy of the system lacks lower-semicontinuity and equilibrium solutions that minimize the energy do not exist in general. In particular, time-incremental formulations suffer from a restart problem, i.e., the incremental problem becomes ill-defined when a microstructure has been previously established in the system and the initial conditions for the future evolution of the system are only defined in the sense of Young measures. However, it is possible characterize entire trajectories of the system as minimizers of certain energy dissipation functionals, thus entirely circumventing the restart problem of the classical rate and time-incremental problems. Because of the minimizing property of the trajectories of the system, tools of the calculus of variations such as the direct method for establishing existence, relaxation and optimal scaling can be applied. Selected examples illustrate how those tools shed light into microstructural evolution and on the effective kinetics governing the macroscopic evolution of the system.

Nanomechanics of Carbon Nanotubes

Traian Dumitrica
Professor
Department of Mechanical Engineering, University of Minnesota

Advances in condensed matter physics and theoretical chemistry have made possible a comprehensive modeling of materials. We can adapt and apply these theoretical methods to study the amazing properties of nanostructures. I will discuss two examples where such theories helped the understanding of the mechanical response of carbon nanotubes (generally viewed as a paradigm for nanoscale materials).

In materials modeling the most common way to implement molecular dynamics is via translational periodic boundary conditions. This is not the natural choice when modeling carbon nanotubes. Using the helical and rotational symmetries of the nanoscale graphitic tubules, molecular dynamics and structural relaxation can be done in a simplified way, on a modest number of atoms. This new method [1], termed objective molecular dynamics [2, 3], is compatible with quantum mechanics under the Born-Oppenheimer approximation. The utility of objective molecular dynamics will be presented in the context of studying the carbon nanotubes under bending and twist.

Combining a probabilistic approach of the rate theory with detailed quantum mechanical computations of failure nucleation and transition-state barriers, allows for a comprehensive analysis of the underlying atomic mechanisms and evaluation of the yield strain for arbitrary nanotubes under realistic conditions [4]. The numerical results are captured in a concise set of equations for the breaking strain, and reveal a competition between two alternative routes of brittle bond breaking and plastic relaxation. The employed probabilistic approach ultimately allows for the creation of a "strength map", which plots the likelihood that a nanotube will break—and how its likely to break.

References

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[2] T. Dumitrica and R.D. James, Objective Molecular Dynamics, Journal of the Mechanics and Physics of Solids 55, 2206 (2007).

[3] D.-B. Zhang, M. Hua, and T. Dumitrica, Stability of Polycrystalline and Wurtzite Si Nanowires via Symmetry-Adapted Tight-Binding Objective Molecular Dynamics, Journal of Chemical Physics 128, 084104 (2008).

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Phonon Analysis of Carbon Nanotubes with Arbitary Chirality by the Objective Structures Framework

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Ryan S. Elliott
Department of Aerospace Engineering and Mechanics, University of Minnesota

Normal modes of vibrations of collections of atoms, called phonons, provide important information about thermodynamic properties of materials. Further, they can be exploited to predict equilibrium crystal structures as a function of temperature and other environmental variables using bifurcation techniques [1,2]. However, computing the normal mode spectrum is extremely expensive, except in the special case of periodic crystals where Fourier techniques simplify the calculation. Recently, R. D. James observed a close analogy between crystals and certain complex atomic structures as well as biological structures [1]. Structures that satisfy this analogy are termed "Objective Structures". They include carbon nanotubes of all chiralities, buckyballs, as well as many biological virus components. This analogy brings in the idea of "Objective Boundary Conditions". The Objective Boundary Conditions allow for the same efficiencies that have made crystalline structures accessible to efficient calculation with periodic boundary conditions (ex. [4]), by allowing treatment of a single unit cell representative of the entire structure. Here, we develop the Objective analog of the Fourier transform to analyze phonon modes in carbon nanotubes. It allows us to treat carbon nanotubes with great efficiency by providing a basis that decouples the modes. Further, previous calculations of phonon spectra apply conventional periodic boundary conditions along the length of the nanotube. Hence chiral nanotubes require very large fundamental domains and the associated large computational cost. The use of the Objective Structures framework allows us to consider very small fundamental domains, regardless of chirality, with minimal computational effort. Further, our efforts are a step toward implementing a framework [1,2] to understand the equilibrium structures of carbon nanotubes under applied loads.

References

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[3] R.D. James, Journal of the Mechanics and Physics of Solids, 54, 2354-2390, 2006.

[4] T. Dumitrica and R. D. James, Journal of the Mechanics and Physics of Solids, 55, 2206-2236, 2007.

Mathematical Foundations and Algorithms for the Quasicontinuum Method

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Professor
School of Math, University of Minnesota

Marcel Arndt
School of Math, University of Minnesota

Matthew Dobson
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We will give an overview of the current state of numerical analysis and algorithms for the quasicontinuum method. We will present results for atomistic-to-continuum coupling error, rates of convergence for iterative solution methods, a posteriori error estimation, and adaptive algorithms for atomistic-continuum modeling and continuuum coarsening.

Thermoplastic Elastomers: Multiscale Modeling and Microstructure Evolution

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Thermoplastic elastomers (TPEs) are block copolymers made up of "hard" (glassy) and "soft" (rubbery) domains that self-organize on a length scale of a few tens of nanometers. Under typical processing conditions, TPEs also develop a "granular" structure at the micron level, which is similar to that of metal polycrystals. Therefore, TPEs can be described as materials with (continuum) heterogeneities at two different length scales. In this talk, we will develop constitutive models for TPEs with lamellar morphology, where the grains are made up of the same, perfect, lamellar structure (single crystal) with randomly varying lamination directions (crystal orientations). In particular, based on experimental evidence, we consider two types of such materials: "oriented" and "unoriented" samples. The oriented TPEs are highly ordered, near-single-crystal systems with slightly varying grain orientations, while the unoriented samples are initially isotropic due to an initially random distribution of orientations in the sample. For oriented TPEs, it is found that under certain loading conditions; namely, under those with sufficiently large compressive deformations applied in the direction of the layers within the individual grains?the overall behavior of the material becomes macroscopically unstable (i.e., it loses strong ellipticity). The unoriented samples are also susceptible to loss of strong ellipticity, especially for large contrast in mechanical properties of the hard and soft domains. Finally, these instabilities will be related to the evolution of the underlying microstructure, which can be tracked experimentally (via small X-ray scattering measurements) in these systems.

High Pressure Mechanochemistry: Multiscale Theory, Experiment, and Search for New Materials

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Yanzhang Ma
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High pressure mechanochemistry studies the effect of large plastic shear on high pressure phase transformations and chemical reactions. We developed rotational diamond anvil cell (RDAC) technique to study in situ strain-induced phase transformations in various material systems [1], including BN, Si, SiC and iron. Synchrotron X-ray diffraction and Raman spectroscopy is used. A three-scale continuum thermodynamic theory and closed form solutions are developed to describe observed mechanochemical phenomena [2,3]. Finite element simulations are performed as well [4]. At the nanoscale, a model for strain-induced nucleation at the tip of a dislocation pile-up is suggested and studied. At the microscale, a simple strain-controlled kinetic equation for the strain-induced phase transformations is thermodynamically derived. It depends (among other parameters) on the ratio of the yield strengths of phases. A macroscale model for plastic flow and strain-induced phase transformations in RDAC is developed and finite element solutions are found. These models explain why and how the superposition of plastic shear on high pressure leads to: a) a significant (by a factor of 3-10) reduction of the phase transformations pressure, b) reduction (up to zero) of pressure hysteresis, c) the appearance of new phases, especially strong phases, which were not obtained without shear, d) pressure growth during phase transformations (despite the volume decrease), and e) strain-controlled (rather than time-controlled) kinetics. Some methods of characterization and controlling the phase transformations are suggested and the unique potential of plastic straining to produce high-strength metastable phases is predicted. Some new phenomena are predicted theoretically and confirmed experimentally. Thus, phase transformations induced by rotational plastic instability was revealed and used to reduce pressure for irreversible phase transformations from hexagonal to superhard cubic BN from 55 GPa to 5.6 GPa [5]. Transformation-induced plasticity was revealed [1] which serves as a positive mechanochemical feedback for intensification of phase transformations.

References

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A Quasicontinuum for Multilattice Phase Transforming Materials

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The quasicontinuum (QC) method [1-2] is applied to materials possessing a multilattice crystal structure. Cauchy-Born (CB) kinematics, which accounts for the shifts of the crystal basis, is used in continuum regions to relate atomic motions to continuum deformation gradients. To avoid failures of the CB kinematics, QC is augmented with a phonon stability analysis that detects lattice period extensions and identifies the minimum required periodic cell size [3]. This augmented approach is referred to as "Cascading Cauchy-Born kinematics". Applications to one- and two-dimensional test problems that highlight the salient features will be presented. In particular, an effective interaction potential material model for a prototypical shape memory alloy is used to simulate a complete shape memory cycle. The results capture both temperature- and stress-induced martensitic transformations.

References

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About Stress-Induced Phase Transformations in Shape-Memory Polycrystals

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Division of Engineering and Applied Science, California Institute of Technology

Above the phase transformation temperature, shape-memory alloys show a superelastic behavior upon an applied stress. This is due to a phase transformation induced by the applied stress. It is interesting to know the onset of stress-induced transformation from a general perspective as well as with respect to applications. Our aim is to determine and study this onset mathematically within the framework of energy minimization and homogenization theory [1].

We study a model case of scalar materials, give appropriate definitions of the transformation yield set in polycrystalline materials and show that the Sachs bound is a sharp bound on the yield set. That is, the Sachs bound turns out to characterize the onset of phase transformation in this case.

Furthermore we derive bounds on stress-strain curves of polycrystalline scalar shape-memory alloys; these bounds are based on an approach by Milton and Serkov [2], which was developed to bound currents in nonlinear conduction composites. To give specific examples, we consider four variant materials with special textures.

References

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Combinatorial Approach to Materials Discovery

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I will describe the applications of the combinatorial approach for rapidly optimizing and fine tuning physical properties of multifunctional materials. In particular, we have applied this technique to search for thermoelastic shape memory alloys with minimal hysteresis widths. Synchrotron microdiffraction was performed on ternary composition spreads of Ni-Ti-Cu in order to track the continuous change in lattice parameters across a large region of the phase diagram mapped on a single Si wafer. A clear relation between the transformation matrix (determined by the lattice parameters) and the thermal hysteresis of the shape memory alloys were observed across a large compositional region which verified the non-linear theory of martensite.

Breaching the Work Output Limitation of Ferromagnetic Shape Memory Alloys

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In recent years, a special class of active materials known as ferromagnetic shape-memory (FSM) alloys has received much attention due its large actuation strains and fast response. Despite of the large strains, the work output of FSM alloys are limited by their relatively low blocking stress of 2-6 MPa, above which magnetic field induced strain is not possible. This level of stress impedes the utilization of these alloys in practical applications where high work output by small components is required. To date, attempts to enhance the work output limitation are mainly focused on changing the concentrations of the off stoichiometric compounds of the FSM alloys, as they set the level of the magnetocrystalline anisotropy energy constant. In this paper we suggest that the work output limitation can be breached by reducing the size of the actuator, and present an indication of a possible fundamental relationship between size and work output capabilities.

Overall, the behavior of FSM alloys involves motion of twin boundaries and is significantly influenced by its microstructure. Based on a theoretical model, we have shown that down-scale specimens have finer twin boundary microstructure that consequently may increase the blocking stress. In light of this, a novel experimental method was realized to establish this conjecture and to provide comprehensive information on the behavior of micro-scale actuators. A series of tests demonstrated no actuation strain reduction up to extraordinary loads of 10MPa, which is we believe to be related to the size reduction of the FSM alloy in our experiments.

An Effective Interaction Potential Model of Stress- and Temperature-Induced Martensitic Transformations in Perfect Bi-atomic Crystals

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Solid-to-solid martensitic phase transformations are technologically important phenomena that result in unique macroscopic material properties such as the shape memory effect, ferromagnetism, and ferroelectric behavior. In shape memory alloys, such as CuAlNi and NiTi, the martensitic transformation can result from a change in temperature or the application of stress. In fact, both temperature-induced and stress-induced transformations are essential for the existence of shape memory behavior.

An Effective Interaction Potential model for bi-atomic shape memory alloys, based on a set of temperature-dependent atomic pair-potentials, is presented. The equilibrium solutions of the governing nonlinear equations are found, as functions of temperature and applied stress, using symmetry arguments and Branch-Following and Bifurcation techniques. To check if a given equilibrium path is observable, its stability against perturbations of arbitrary (with respect to interatomic distance) wavelengths is investigated. This requires continuum-level energy calculations as well as a lattice-level phonon spectra analysis. Our work predicts the existence of a hysteretic two-step temperature-induced proper martensitic transformation from the high-temperature B2 cubic austenite phase, to an intermediate alpha-IrV orthorhombic phase, to a final B19 orthorhombic martensite phase. Stress-induced transformation to the alpha-IrV phase is predicted, at high temperatures, and characteristic properties such as tension-compression asymmetry are captured. Additionally, the transformation stress is found to increase with increasing temperature in agreement with experiment. The existence of both temperature- and stress-induced transformations indicates the possibility for shape memory behavior. Finally, the predicted transformation parameters show good correspondence with experimental values for the shape memory alloys CuAlNi and AuCd.

Nanoscale Piezoelectricity

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Crystalline piezoelectric dielectrics electrically polarize upon application of uniform mechanical strain. Inhomogeneous strain, however, locally breaks inversion symmetry and can potentially polarize even non-piezoelectric (centrosymmetric) dielectrics. Flexoelectricty—the coupling of strain gradient to polarization— is expected to show a strong size-dependency due to the scaling of stain gradients with structural feature size. In this study, using a combination of atomistic and theoretical approaches, we investigate the "effective" size-dependent piezoelectric and elastic behavior of inhomogeneously strained non-piezoelectric and piezoelectric nanostructures. We argue, through computational examples, the tantalizing possibility of creating "apparently piezoelectric" nano-composites without piezoelectric constituents. Further, to obtain analytical results and tease out the novel physical insights, we analyze a paradigmatic nanoscale cantilever beam. We find that in materials that are intrinsically piezoelectric, the flexoelectricity and piezoelectricity effects do not add linearly and exhibit a nonlinear interaction. The latter leads to a strong size-dependent enhancement of the apparent piezoelectric coefficient resulting in, for example, a "giant" 500% enhancement over bulk properties in $BaTiO_3$ for a beam thickness of 5 nm. Correspondingly, for non-piezoelectric materials also, the enhancement is non-trivial (e.g. 80 % for 5 nm size in paraelectric $BaTiO_3$ phase). Flexoelectricity also modifies the apparent elastic modulus of nanostructures, exhibiting an asymptotic scaling of $1/h^2$ where "h" is the characteristic feature size. Our major predictions are verified by quantum mechanically derived force-field based molecular dynamics for two phases (cubic and tetragonal) of $BaTiO_3$.

Stability of Shape Memory Alloy Honeycomb under Finite-Strain Isothermal Compression Cycles of Various Amplitudes

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Metallic foams and honeycombs, with their light-weight, high specific stiffness, and well-developed energy absorption characteristics, are of obvious utility in engineering applications. However, these structures, often made of aluminum, suffer permanent deformation after crushing. Cellular structures made from shape-memory alloys (SMAs) are particularly intriguing for their potential to deliver shape memory and/or superelasticity in a light-weight material. Realization of open-celled Nitinol has recently become possible via a (newly discovered by Profs. D. Grummon at Michigan State Univ. and J. Shaw at Univ. of Michigan) transient-liquid reactive brazing system for creating robust metallurgical Nitinol-Nitinol bonds. With this technique, prototype sparse cellular honeycomb structures have been made and tested, showing up to 50% repeatedly recoverable strains.

Of particular interest here, in addition to modeling experiments on SMA's, is an in-depth investigation of the isothermal, hysteretic response of these honeycomb materials and the stability of their deformation patterns at finite strains. A detailed investigation of the influence of the material constitutive law on the macroscopic stress-strain behavior of these honeycombs is presented. It is found that instabilities—in the form of departure from the principal solution where all cells deform in the same pattern—appear with the increase of macroscopic strains as the cell-wall alloy transforms from austenite to martensite and then eventually disappear, upon further macroscopic straining, as all the cell-wall alloy is all in the martensitic phase. Upon unloading, where the cell-wall alloy material reverses this transformation, similar instabilities appear and disappear. The stability of honeycomb structure is addressed i) by using one-cell Bloch wave calculations for the infinite perfect case, ii) by using large perfect-geometry samples to account for specimen boundary conditions and finally iii) by using large imperfect-geometry samples to compare and contrast with experimental results.

Some Two-Phase Problems of Nonlinear Elasticity in the Presence of Small Interfacial Energy: A Global Bifurcation Approach

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We consider several different physical problems, having a common mathematical structure: a non-convex energy in the lower-order terms plus a higher-order regularization (or singular perturbation), the latter characterized by a small parameter (or parameters). We study the equilibria of such systems, focusing on local minima of the total energy. We propose a novel approach based upon techniques of global bifurcation and a-priori bounds—with the reciprocal of the small parameter playing the role of a "large" continuation parameter. We indicate applications to shape-memory solids, thin flexible sheets and lipid bi-layer membranes.

Transmission Electron Microscopy Studies of Novel Ni-Ti-based Shape Memory Alloys

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The quest for new shape memory alloys better suited for particular applications usually follows a path where numerous extra constituents are added to the basic alloys in smaller or larger amounts. Though the choice of elements and ratios is normally based on their known effects in similar systems, this approach is essentially still trial-and-error based. Recently, a new approach has been suggested by R. James et al. in which a dedicated search for alloys with a low hysteresis was coupled with measurements of the austenite-martensite transformation matrix [1]. A low or zero hysteresis is expected when the middle eigenvalue lambda2 of this transformation matrix equals 1. At the same time, this condition implies a perfect fit at the habit plane so that no microtwinning in the martensite is necessary. Moreover, this condition also divides the remaining phase space into two parts, one with Type I and II twins (lambda2 > 1) and one with compound twins (lambda2 < 1). One such system is Ni-Ti-Pd in which Ni is replaced by Pd.

The present contribution focuses on transmission electron microscopy (TEM) work of Ni-Ti-Pd alloys with different compositions with lambda2 varying around 1. The TEM micrographs clearly confirm the existence of Type I and II twins at lambda2 > 1 with a decreasing twin density when approaching lambda2 = 1. In one sample, a twinless habit plane could be observed to grow during an in-situ cooling experiment. However, on some occasions also compound twins are observed in samples with lambda2 > 1.

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Mechanics of NiTi Fatigue for Vascular Stent Design

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Nitinol has become a frequently used medical implant material despite its notorious complexity, especially with respect to fatigue [1]. This intermetallic compound, NiTi, when designed & manufactured into a femoral arterial stent is able to spring out of a intra-vascular catheter, hold the diseased artery open, and undergo millions of cycles of large deformation due to walking, sitting-standing, et cetra without failure, usually. This talk will elucidate how mechanics is used to measure and model the use conditions in-vivo, and the fatigue life of a NiTi stent.

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